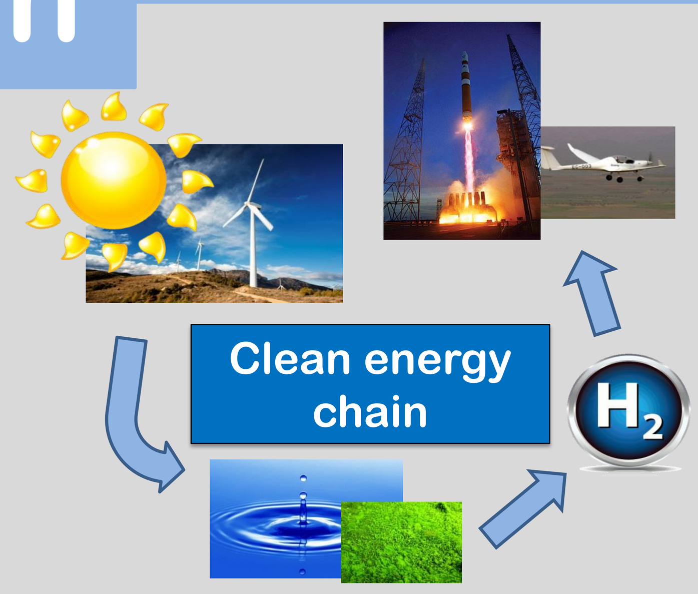
Hydrogen Energy Research in the Department of Chemical Engineering, University of Bath, UK

Nuno Bimbo, Simon Owens, Jessica Sharpe, Antonio Noguera, Andrew Rushworth, Matthew Smith, Michael Berry, Phoebe Hayes and Timothy Mays.

URL: http://people.bath.ac.uk/cestjm

Hydrogen

- Highest energy content of any chemical fuel on a mass basis
- Is abundant in the form of water, biomass or hydrocarbons
- If combusted or used in a fuel cell with pure oxygen, its only product is water
- Can be used as a wide-scale clean energy vector



Hydrogen storage

- A very low density gas (0.08988 g/L), liquid (31.26 to 77.01 g/L) and solid (87.08 g/L)
- Challenge is to increase volumetric density so it can be used for mobile applications
- One storage solution is to use highly porous materials for hydrogen storage

Hydrogen isotope separation

- Palladium stores large amounts of hydrogen isotopes at NTP and is therefore a popular means of separating hydrogen isotopes
- Hydrogen isotope exchange occurs in palladium during isotope separation processes
- Challenge is to understand kinetics and mechanisms of isotope exchange

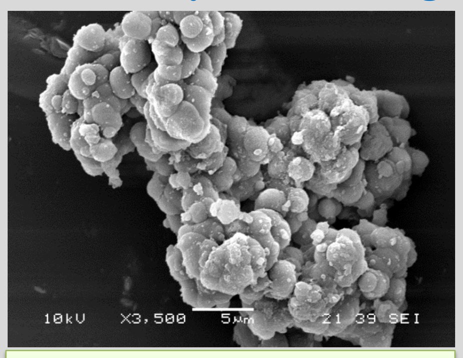
Equipment

Clockwise from top left: X-ray diffractometer; IsoEx apparatus, Thermal Gravimetric analyser, HTP-1 volumetric sorption analyser, ASAP 2020 sorption analyser (centre), Helium pycnometer and IGA gravimetric sorption analyser

Hydrogen Storage in Porous Materials

Materials

Polymers of intrinsic microporosity



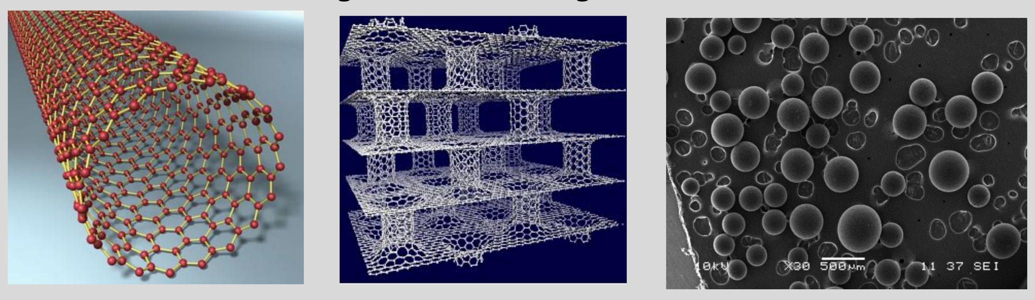
SEM of PIM-1

- High surface areas (~6500 $m^2\ g^{-1}$)
- Tunable materials
- Superior stability

Carbons

Advantages:

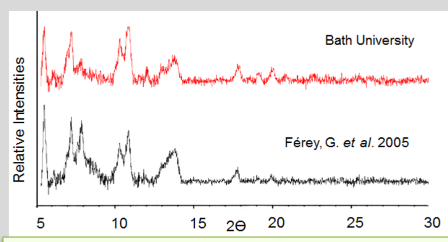
- Reversible, lightweight and cheap
- Wide variety of structural forms
- Good thermal stability
- Ability to modify the structure



Nanotube, Pillared Graphene, carbon beads

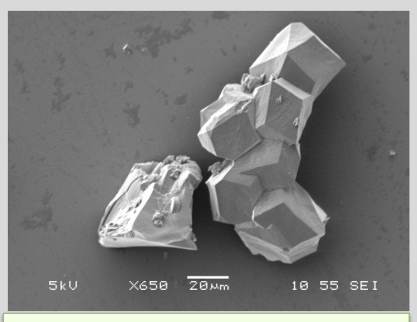
Examples: Activated carbons, Nanotubes, Graphite, Pillared Graphene

Metal-organic frameworks

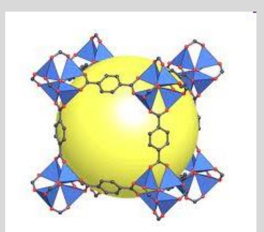


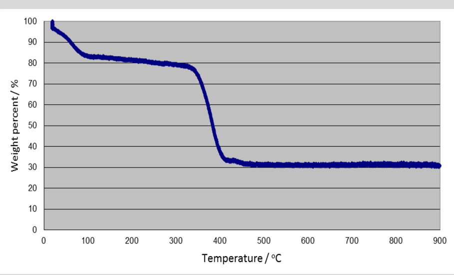
MIL-101(Cr) XRD

- Metal centres strongly bonded to organic linkers
- High surface area
- Highly tunable
- Highest H_2 uptake so far



SEM of MOF-177

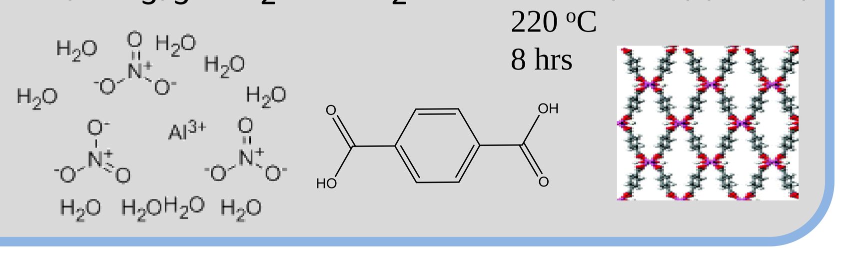




MIL-101(Cr) TGA

Example synthesis:

$Al(NO_3)_3.9H_2O + H_2BDC \xrightarrow[220\,^{\circ}C,\ 8\,hrs]{H_2O} Al(OH)(BDC)$



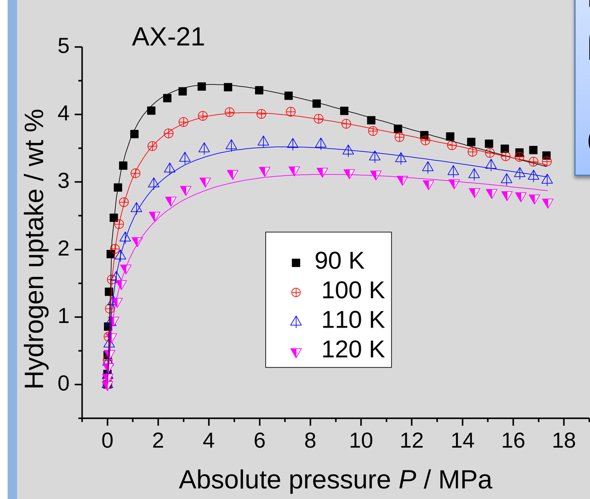
Results

Analysis

- Analysis and modelling of excess isotherms to compare with alternative storage methods

$m_E = (\rho_A - \rho_B) V_P \theta_A$

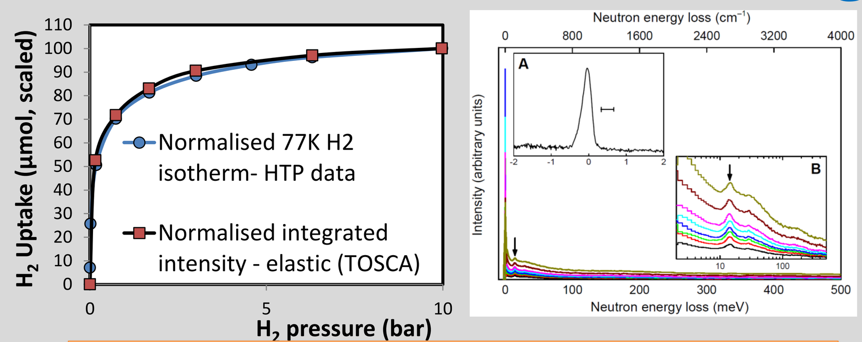
m_E = excess uptake
ρ_A = adsorbate density
ρ_B = bulk density
V_P = pore volume
Θ_A = fill factor



This allows us to determine the optimum conditions for physisorption

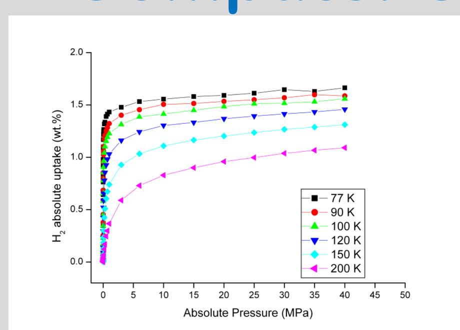
Experimental high-pressure hydrogen excess and fitted isotherms for AX-21

Inelastic neutron scattering



INS integrated elastic peak and spectra for TE7

Computer simulations



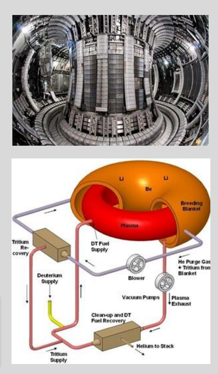
Simulated isotherms for Silicalite-1 using MUSIC

Hydrogen Isotope Separation

- Palladium forms a non-stoichiometric interstitial hydride when exposed to hydrogen or deuterium
  - $PdH_{0.7}$ @ 1 bar, 300K
  - $PdD_{0.65}$ @ 1 bar, 300K

Pd powder

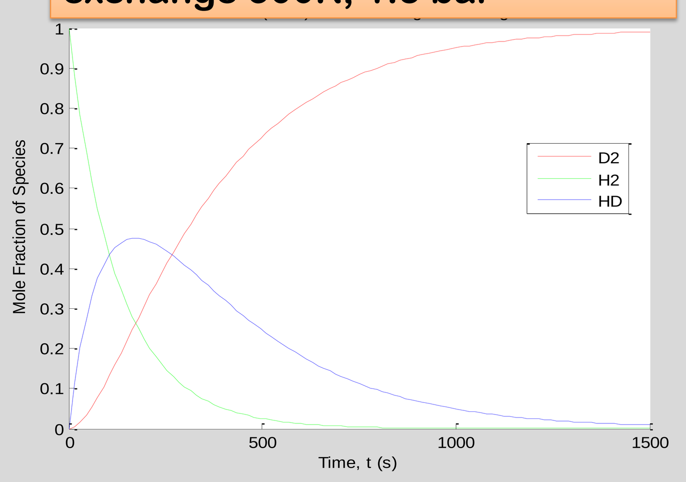
- Exchange Reaction:
  - $H_2\,(g) + D_s \longleftrightarrow HD\,(g) + H_s$ $[D_s = PdD_x]$
  - $HD\,(g) + D_s \longleftrightarrow D_2\,(g) + H_s$ $[H_s = PdH_x]$
- Both exchange directions can occur:
  - PdD_x to PdH_y
  - PdH_x to PdD_y



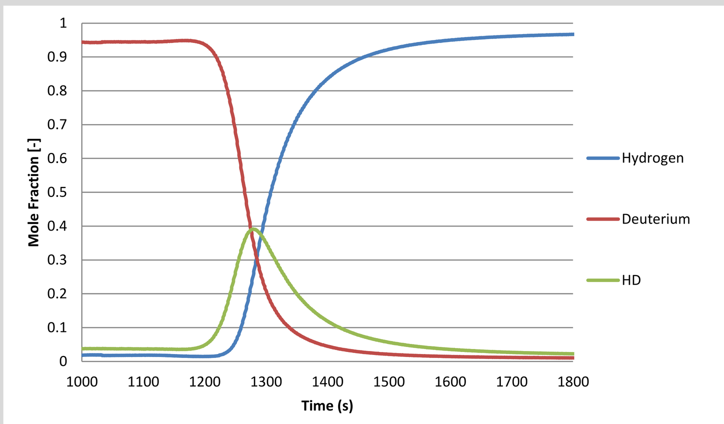
ITER

Analysis

MATLAB Simulated PdH to PdD exchange 300K; 1.5 bar

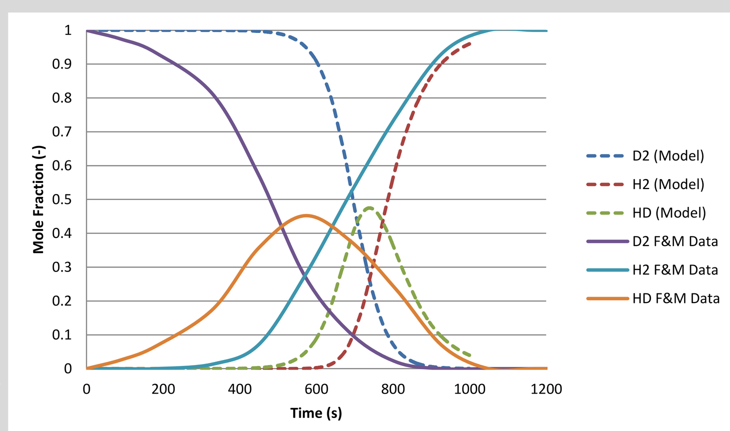


Experimental



Experimental PdD to PdH exchange @ 293K; 1.5 bar

- Modelling performed on:
  - COMSOL
  - MATLAB
  - 1D MATLAB
  - 2D/3D COMSOL



COMSOL Simulated PdD to PdH exchange 300K; 1.5 bar

Phoebe, Andrew, Jess, Nuno, Tim, Antonio, Matthew, Simon and Michael

EPSRC Pioneering research and skills

Centre for Sustainable Chemical Technologies

Department of Chemical Engineering
University of Bath